Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:28 PM GMT

PDB ID	:	4F4K
Title	:	DNA Polymerase I Large Fragment Complex 6
Authors	:	Wang, W.; Beese, L.S.
Deposited on	:	2012-05-10
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

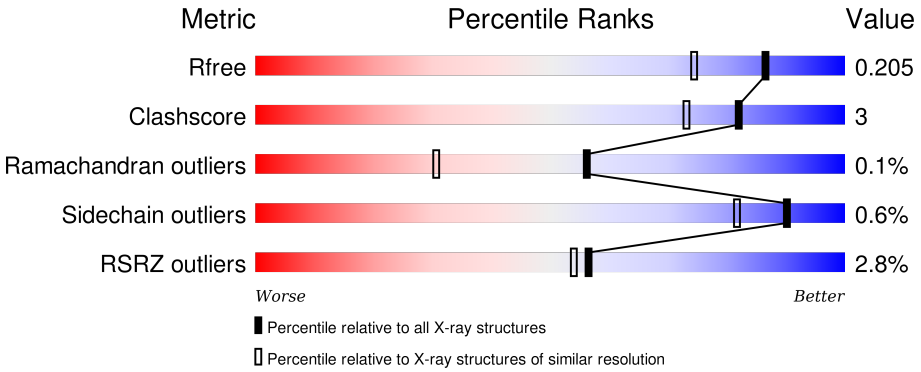
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	592	4%, 90%, 8%
1	D	592	2%, 91%, 6%
2	B	9	44%, 44%, 11%
2	E	9	33%, 56%, 11%
3	C	13	38%, 31%, 15%, 15%

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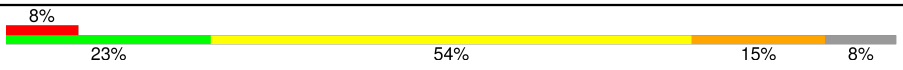
Mol	Chain	Length	Quality of chain
3	F	13	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21725 atoms, of which 10028 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	579	Total	C	H	N	O	S	0	6	0
			9450	2979	4768	814	872	17			
1	D	579	Total	C	H	N	O	S	0	10	0
			9484	2992	4787	810	877	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
A	710	TYR	PHE	ENGINEERED MUTATION	UNP Q5KWC1
A	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1
D	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
D	710	TYR	PHE	ENGINEERED MUTATION	UNP Q5KWC1
D	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1

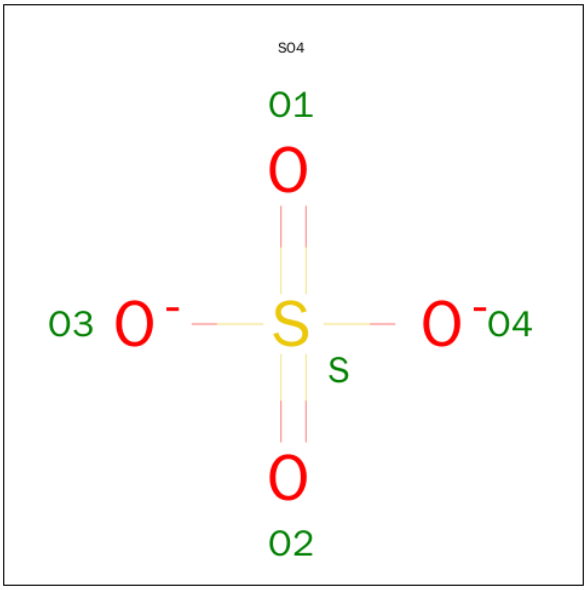
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DDG))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			277	86	100	31	52	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			277	86	100	31	52	8			

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*TP*TP*CP*GP*AP*GP*TP*CP*AP*GP*G)-3').

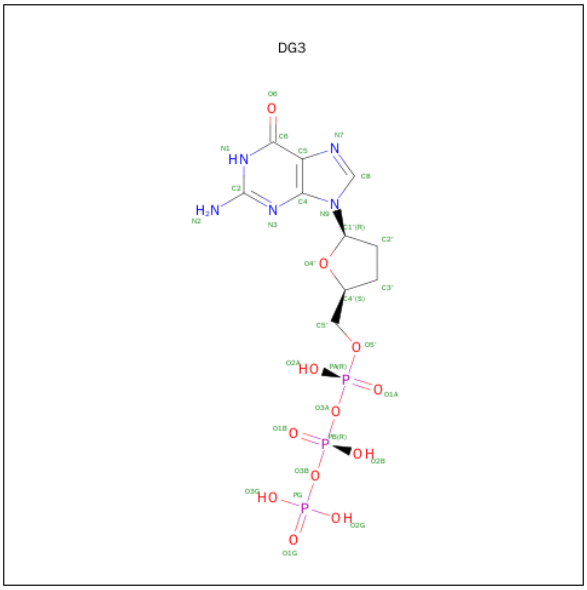
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	11	Total	C	H	N	O	P	0	0	0
			352	108	124	42	67	11			
3	F	12	Total	C	H	N	O	P	0	0	0
			381	118	135	47	70	11			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DG3) (formula: $C_{10}H_{16}N_5O_{12}P_3$).

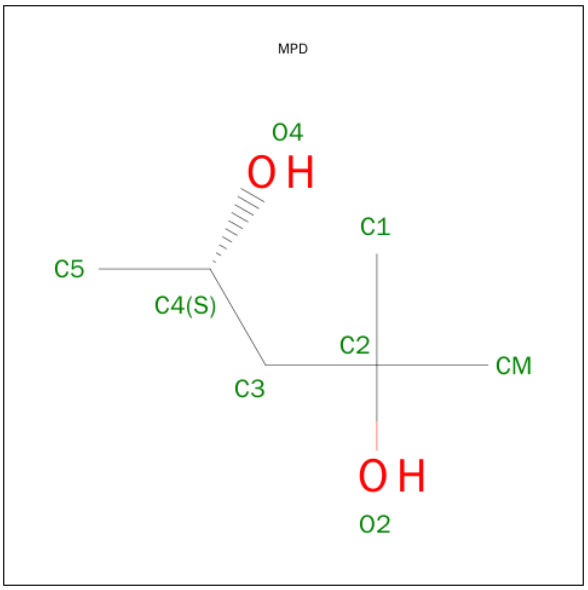


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mn	0	0
			1	1		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	493	Total	O	0	0
			493	493		
8	C	60	Total	O	0	0
			60	60		
8	D	735	Total	O	0	0
			735	735		
8	B	37	Total	O	0	0
			37	37		

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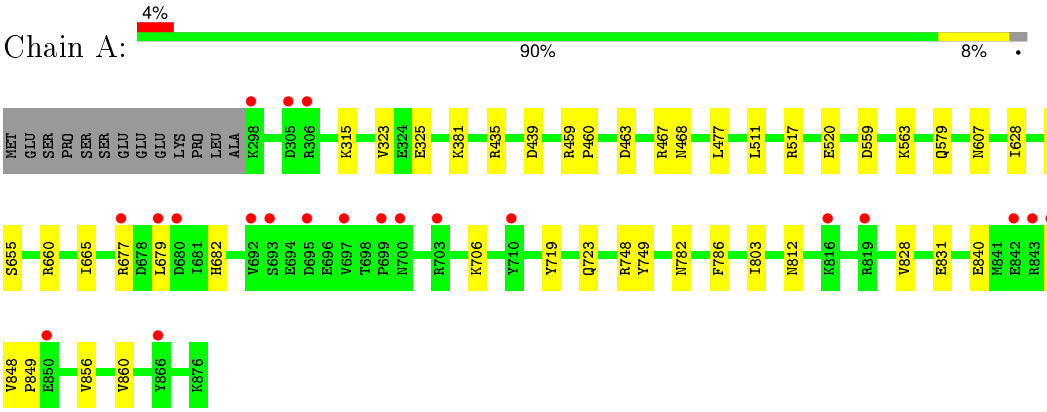
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	77	Total O 77 77	0	0
8	E	34	Total O 34 34	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

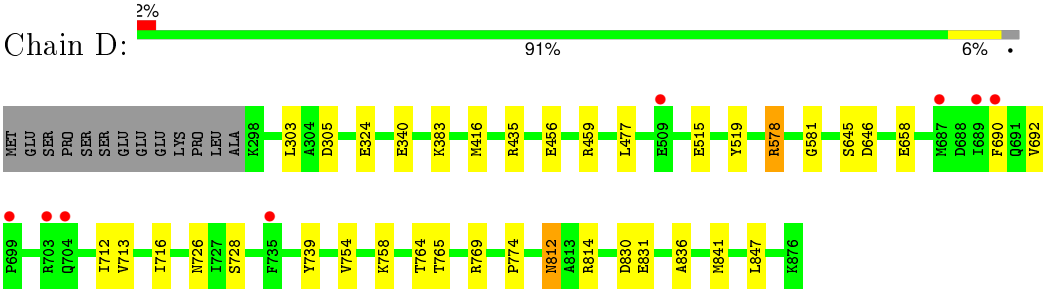
- Molecule 1: DNA polymerase

Chain A:



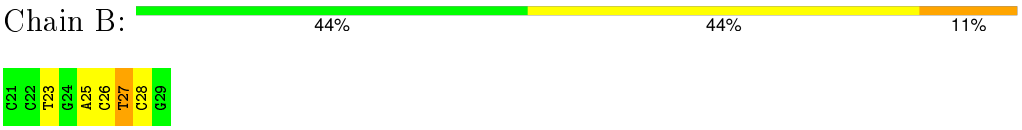
- Molecule 1: DNA polymerase

Chain D:



- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DDG))-3')

Chain B:



- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DDG))-3')

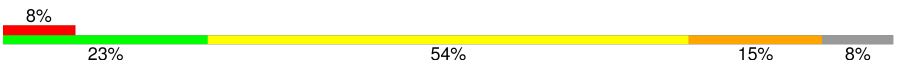
Chain E:

- Molecule 3: DNA (5'-D(*CP*AP*TP*TP*CP*GP*AP*GP*TP*CP*AP*GP*G)-3')

Chain C:

• Molecule 3: DNA (5'-D(*CP*AP*TP*TP*CP*GP*AP*GP*TP*CP*AP*GP*G)-3')

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.81Å 109.22Å 150.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.06 – 1.60 61.99 – 1.60	Depositor EDS
% Data completeness (in resolution range)	88.2 (30.06-1.60) 88.2 (61.99-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, R_{free}	0.171 , 0.194 0.183 , 0.205	Depositor DCC
R_{free} test set	8168 reflections (4.77%)	DCC
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.75$, $< L^2 > = 0.66$	Xtriage
Outliers	248 of 179465 reflections (0.138%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21725	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DG3, MPD, MN, DDG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.42	0/4784	0.56	0/6464
1	D	0.59	0/4812	0.69	3/6503 (0.0%)
2	B	1.07	0/173	1.79	8/264 (3.0%)
2	E	1.16	1/173 (0.6%)	1.90	6/264 (2.3%)
3	C	1.10	1/255 (0.4%)	2.08	14/392 (3.6%)
3	F	1.11	0/276	1.89	9/425 (2.1%)
All	All	0.59	2/10473 (0.0%)	0.84	40/14312 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	25	DA	C3'-O3'	-5.39	1.36	1.44
3	C	5	DG	C3'-O3'	5.02	1.50	1.44

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	578	ARG	NE-CZ-NH2	-10.85	114.88	120.30
3	F	8	DT	O4'-C1'-N1	-10.80	100.44	108.00
1	D	578	ARG	NE-CZ-NH1	8.92	124.76	120.30
3	C	8	DT	O4'-C1'-N1	-8.80	101.84	108.00
2	E	23	DT	O4'-C1'-N1	-8.58	101.99	108.00
3	C	5	DG	C5-C6-N1	-8.57	107.22	111.50
3	F	2	DT	O4'-C1'-N1	8.46	113.92	108.00
3	C	5	DG	C2-N3-C4	-8.29	107.75	111.90
2	E	27	DT	O4'-C4'-C3'	-8.26	101.05	106.00
3	C	11	DG	O4'-C1'-N9	-8.10	102.33	108.00
3	C	5	DG	N3-C4-N9	-7.89	121.27	126.00
3	F	11	DG	O4'-C1'-N9	-7.58	102.69	108.00
3	C	5	DG	C6-N1-C2	7.15	129.39	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	23	DT	N3-C4-O4	7.14	124.18	119.90
2	E	26	DC	O4'-C1'-N1	6.41	112.49	108.00
3	C	5	DG	N3-C4-C5	6.17	131.69	128.60
3	F	3	DT	C6-C5-C7	-6.06	119.27	122.90
3	F	6	DA	OP1-P-OP2	-5.94	110.69	119.60
2	B	27	DT	O4'-C1'-N1	5.78	112.05	108.00
2	B	26	DC	O4'-C1'-N1	5.77	112.04	108.00
2	B	28	DC	C2-N3-C4	5.75	122.78	119.90
2	B	23	DT	C5-C4-O4	-5.75	120.88	124.90
2	B	23	DT	O4'-C1'-N1	-5.73	103.99	108.00
3	C	7	DG	C2-N3-C4	5.67	114.74	111.90
2	B	25	DA	O4'-C1'-C2'	5.62	110.40	105.90
3	C	3	DT	N3-C4-O4	5.60	123.26	119.90
3	C	2	DT	O4'-C1'-N1	5.58	111.90	108.00
3	C	3	DT	C5-C4-O4	-5.49	121.06	124.90
2	B	27	DT	O4'-C4'-C3'	-5.40	102.34	104.50
3	F	5	DG	C5-N7-C8	-5.31	101.64	104.30
3	C	7	DG	C6-C5-N7	5.29	133.57	130.40
2	E	26	DC	N1-C1'-C2'	-5.27	102.58	112.60
2	E	28	DC	C4'-C3'-C2'	-5.24	98.38	103.10
3	F	4	DC	O5'-P-OP2	-5.24	100.99	105.70
3	C	11	DG	C2-N3-C4	-5.22	109.29	111.90
2	E	23	DT	C5-C4-O4	-5.16	121.29	124.90
3	F	10	DA	O4'-C1'-N9	-5.04	104.47	108.00
1	D	830	ASP	CB-CG-OD2	-5.01	113.79	118.30
3	F	4	DC	C4-C5-C6	5.01	119.91	117.40
3	C	7	DG	C5-C6-N1	5.01	114.00	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4682	4768	4757	26	0
1	D	4697	4787	4775	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	177	100	103	2	0
2	E	177	100	103	2	0
3	C	228	124	125	2	0
3	F	246	135	137	2	0
4	A	5	0	0	0	0
4	D	10	0	0	0	0
5	D	30	0	12	3	0
6	D	1	0	0	0	0
7	D	8	14	14	0	0
8	A	493	0	0	10	0
8	B	37	0	0	3	0
8	C	60	0	0	2	0
8	D	735	0	0	14	0
8	E	34	0	0	0	0
8	F	77	0	0	0	0
All	All	11697	10028	10026	64	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:901:DG3:HN1	3:F:3:DT:H3	1.12	0.96
2:B:27:DT:OP2	8:B:230:HOH:O	1.90	0.88
1:D:812[A]:ASN:OD1	8:D:1178:HOH:O	1.91	0.88
1:D:416:MET:HE3	8:D:1689:HOH:O	1.72	0.88
2:B:27:DT:OP1	8:B:237:HOH:O	1.91	0.87
3:C:3:DT:O4	8:C:151:HOH:O	1.94	0.83
1:D:340:GLU:OE2	8:D:1702:HOH:O	2.06	0.72
1:D:305:ASP:OD1	8:D:1704:HOH:O	2.11	0.68
1:A:860:VAL:O	8:A:1402:HOH:O	2.13	0.66
1:D:764[B]:THR:HG21	8:D:1596:HOH:O	1.97	0.64
1:A:655:SER:O	1:A:660:ARG:NH1	2.30	0.63
1:D:814:ARG:NH2	1:D:847[A]:LEU:HD13	2.18	0.59
1:A:323:VAL:HG12	1:A:435:ARG:NH1	2.18	0.58
1:D:831:GLU:OE2	8:D:1102:HOH:O	2.17	0.58
1:D:456:GLU:HG3	8:D:1722:HOH:O	2.04	0.57
1:D:658:GLU:CD	5:D:901:DG3:H2'1	2.25	0.55
1:A:812[B]:ASN:ND2	8:A:1433:HOH:O	2.33	0.55
1:D:754:VAL:HG12	1:D:758:LYS:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:754:VAL:CG1	1:D:758:LYS:HE2	2.38	0.54
1:D:774:PRO:HA	8:D:1654:HOH:O	2.08	0.53
1:A:677:ARG:HB2	1:A:679:LEU:HG	1.89	0.52
1:A:463:ASP:O	1:A:467[B]:ARG:HG3	2.09	0.52
1:D:713:VAL:HG12	1:D:739[B]:TYR:OH	2.10	0.51
1:D:459:ARG:NH2	8:D:1503:HOH:O	2.43	0.51
1:D:581:GLY:HA3	8:D:1323:HOH:O	2.11	0.51
1:D:435:ARG:NH2	8:D:1347:HOH:O	2.43	0.51
1:A:381:LYS:HE3	8:A:1474:HOH:O	2.10	0.50
1:D:713:VAL:CG1	1:D:739[B]:TYR:OH	2.60	0.50
1:A:665:ILE:HG22	1:A:749:TYR:CE1	2.47	0.50
1:D:726:ASN:HB2	8:D:1466:HOH:O	2.12	0.49
1:A:559:ASP:OD2	1:A:563:LYS:HE2	2.11	0.49
1:A:315:LYS:NZ	8:A:1430:HOH:O	2.39	0.49
1:A:517:ARG:NH1	1:A:520:GLU:OE1	2.46	0.49
1:D:764[B]:THR:HG23	1:D:769:ARG:O	2.13	0.48
1:D:515:GLU:HG2	1:D:519:TYR:CE2	2.49	0.47
1:A:468:ASN:HA	8:A:1363:HOH:O	2.12	0.47
1:A:325:GLU:OE1	8:A:1399:HOH:O	2.20	0.47
1:D:578:ARG:HD3	2:E:26:DC:OP1	2.14	0.47
3:C:11:DG:OP1	8:C:158:HOH:O	2.21	0.46
1:A:631:GLU:OE2	1:A:635:LYS:NZ	2.43	0.45
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.98	0.45
1:A:607[A]:ASN:OD1	8:A:1483:HOH:O	2.21	0.44
1:D:814:ARG:CZ	1:D:847[A]:LEU:CD1	2.95	0.44
1:A:782:ASN:O	1:A:786:PHE:HD2	2.00	0.44
1:D:764[B]:THR:HG22	1:D:765:THR:N	2.33	0.43
1:D:324:GLU:HG2	8:D:1582:HOH:O	2.18	0.43
1:A:682:HIS:CE1	1:A:706:LYS:HD3	2.54	0.43
1:A:579:GLN:HG2	8:B:233:HOH:O	2.18	0.43
3:F:9:DC:H2"	3:F:10:DA:C8	2.53	0.42
1:D:764[B]:THR:HG22	1:D:765:THR:H	1.84	0.42
5:D:901:DG3:O4'	2:E:29:DDG:H2"	2.19	0.42
1:D:836:ALA:HB3	1:D:841:MET:CE	2.50	0.42
1:A:840:GLU:O	1:A:844:LEU:HD13	2.20	0.42
1:D:645:SER:O	1:D:646:ASP:HB2	2.20	0.42
1:A:748:ARG:HG3	8:A:1426:HOH:O	2.20	0.42
1:A:439:ASP:HB3	8:A:1485:HOH:O	2.20	0.41
1:A:803:ILE:HG12	1:A:856:VAL:HG21	2.01	0.41
1:D:383:LYS:HE3	8:D:1442:HOH:O	2.19	0.41
1:D:712:ILE:HA	1:D:716:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:690:PHE:O	1:D:692:VAL:HG13	2.21	0.41
1:A:459:ARG:HB3	1:A:460:PRO:HD3	2.03	0.41
1:A:719:TYR:O	1:A:723:GLN:HG2	2.21	0.41
1:A:828:VAL:HB	1:A:831:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	583/592 (98%)	570 (98%)	12 (2%)	1 (0%)	52 28
1	D	587/592 (99%)	576 (98%)	11 (2%)	0	100 100
All	All	1170/1184 (99%)	1146 (98%)	23 (2%)	1 (0%)	56 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	501/507 (99%)	499 (100%)	2 (0%)	93 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	505/507 (100%)	500 (99%)	5 (1%)	82 67
All	All	1006/1014 (99%)	999 (99%)	7 (1%)	90 78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	477	LEU
1	A	511	LEU
1	D	303	LEU
1	D	477	LEU
1	D	728	SER
1	D	812[A]	ASN
1	D	812[B]	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DDG	B	29	3,2	15,23,24	1.41	2 (13%)	14,33,36	2.33	2 (14%)
2	DDG	E	29	3,2	15,23,24	1.41	2 (13%)	14,33,36	1.75	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DDG	B	29	3,2	-	0/3/18/19	0/3/3/3
2	DDG	E	29	3,2	-	0/3/18/19	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	29	DDG	C8-N7	-2.60	1.29	1.34
2	B	29	DDG	C2-N2	2.97	1.36	1.32
2	E	29	DDG	C2-N2	3.27	1.37	1.32
2	B	29	DDG	C6-N1	3.27	1.41	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	29	DDG	N2-C2-N1	-2.00	115.61	117.80
2	B	29	DDG	N1-C2-N3	2.33	124.91	121.79
2	E	29	DDG	C6-N1-C2	5.08	123.07	120.20
2	B	29	DDG	C6-N1-C2	7.74	124.57	120.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	29	DDG	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	901	-	4,4,4	0.14	0	6,6,6	0.34	0
5	DG3	D	901	6	24,32,32	1.74	2 (8%)	31,50,50	1.86	10 (32%)
4	SO4	D	903	-	4,4,4	0.24	0	6,6,6	0.38	0
4	SO4	D	904	-	4,4,4	0.10	0	6,6,6	0.07	0
7	MPD	D	905	-	6,7,7	0.31	0	7,10,10	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	901	-	-	0/0/0/0	0/0/0/0
5	DG3	D	901	6	-	0/18/31/31	0/3/3/3
4	SO4	D	903	-	-	0/0/0/0	0/0/0/0
4	SO4	D	904	-	-	0/0/0/0	0/0/0/0
7	MPD	D	905	-	-	0/5/5/5	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	901	DG3	C2-N2	4.59	1.43	1.34
5	D	901	DG3	O6-C6	6.13	1.39	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	901	DG3	C1'-N9-C4	-3.57	121.10	127.16
5	D	901	DG3	C5-C6-N1	-3.10	119.36	123.59
5	D	901	DG3	O4'-C1'-C2'	-3.01	103.41	106.67
5	D	901	DG3	C2'-C1'-N9	-2.79	106.83	112.49
5	D	901	DG3	N3-C2-N1	-2.65	123.41	127.44
5	D	901	DG3	C6-C5-C4	-2.62	117.76	120.90
5	D	901	DG3	C3'-C2'-C1'	2.10	105.06	102.71
5	D	901	DG3	O2B-PB-O3B	2.11	114.68	105.09
5	D	901	DG3	C6-N1-C2	3.01	120.12	115.94
5	D	901	DG3	O4'-C1'-N9	3.39	113.58	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	901	DG3	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	579/592 (97%)	0.11	23 (3%) 42 39	14, 32, 58, 91	0
1	D	579/592 (97%)	-0.10	10 (1%) 73 71	7, 20, 38, 51	0
2	B	8/9 (88%)	-0.37	0 100 100	19, 23, 40, 48	0
2	E	8/9 (88%)	-0.49	0 100 100	14, 21, 40, 49	0
3	C	11/13 (84%)	-0.35	0 100 100	16, 23, 40, 59	0
3	F	12/13 (92%)	0.06	1 (8%) 14 12	11, 21, 45, 56	0
All	All	1197/1228 (97%)	-0.00	34 (2%) 56 54	7, 25, 51, 91	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	679	LEU	6.1
1	A	692	VAL	5.4
1	A	703	ARG	5.4
1	A	846	ARG	5.2
1	A	842	GLU	4.2
1	A	298	LYS	4.0
1	D	689	ILE	4.0
1	D	735	PHE	4.0
1	A	816	LYS	3.8
1	A	819	ARG	3.7
1	D	699	PRO	3.7
1	A	305	ASP	3.7
3	F	1	DA	3.5
1	D	703	ARG	3.5
1	A	695	ASP	3.2
1	A	700	ASN	3.0
1	A	693	SER	3.0
1	A	699	PRO	2.9
1	D	704	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	845	CYS	2.9
1	D	509	GLU	2.8
1	A	866	TYR	2.7
1	A	680	ASP	2.7
1	D	695	ASP	2.6
1	A	844	LEU	2.6
1	D	690	PHE	2.6
1	A	697	VAL	2.4
1	A	306	ARG	2.4
1	D	687	MET	2.3
1	A	850	GLU	2.2
1	A	677	ARG	2.1
1	A	843	ARG	2.1
1	D	693	SER	2.1
1	A	710	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	DDG	E	29	21/22	0.98	0.09	-	9,12,16,17	0
2	DDG	B	29	21/22	0.97	0.07	-	18,20,29,29	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	MPD	D	905	8/8	0.92	0.13	1.41	37,52,63,63	0
5	DG3	D	901	30/30	0.95	0.10	-0.05	13,18,22,23	0
4	SO4	A	901	5/5	0.94	0.10	-0.07	33,34,40,46	0
6	MN	D	902	1/1	1.00	0.06	-5.00	17,17,17,17	0
4	SO4	D	903	5/5	0.99	0.07	-	29,30,39,42	0
4	SO4	D	904	5/5	0.96	0.21	-	49,50,55,59	0

6.5 Other polymers (i)

There are no such residues in this entry.